The Computational Toxicology Program in the Office of Research and Development

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The U.S. Environmental Protection Agency (U.S. EPA) is facing increasingly greater demands to develop more efficient and effective methods to evaluate the hazards and risks of chemicals to human health and the environment. To address this need, the ORD has launched a new research program titled Computational Toxicology. Computational Toxicology is defined in the "Framework for a Computational Toxicology Research Program" (see www.epa.gov/comptox) as the application of mathematical and computer models and molecular biological approaches to improve the Agency's prioritization of data requirements and risk assessments. The program traces its origins to a Congressional reprogramming action in FY02, which directed the Agency to conduct research to explore the use of alternatives to animals in testing. In response to that, several proof-of-concept studies for endocrine disruption were undertaken, as it was felt that the U.S. EPA already had a strong research presence in the area and that considerable information was known about the relevant toxicity pathways. Over the past several years, the program has grown in size and importance. This year, the ORD institutionalized the effort by creating the National Center for Computational Toxicology at its campus in Research Triangle Park, NC. The Center is being staffed with systems biologists, computational chemists, and bioinformaticians and will be the focal point for computational toxicology efforts across the ORD. One of the main early challenges of the program will be to develop approaches for prioritizing chemical lists of concern to the Agency for screening and testing purposes. Ideally, this will lead to tailored testing schemes for environmental stressors and to the more effective and efficient use of animals in research. This, in turn, will lead to improved risk assessment methodologies and outcomes. A key part of the program will be development of partnerships with outside organizations that we facilitate and the ensuing discussion of key research needs. This presentation will provide the rationale for creation of the program, highlight some examples of ongoing research related to prioritization and information technology, and suggest parallels between the needs to understand toxicity pathways and to promote sustainable use of chemicals.